Gauge dependence and matching procedure of a nonrelativistic QCD boundstate formalism [a]

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We investigate gauge dependence of a nonrelativistic boundstate formalism used in contemporary calculations. It is known that the effective Hamiltonian of the boundstate system depends on the choice of gauge. We obtain the gauge transformation charge of the Hamiltonian, by which gauge independence of the mass spectrum and gauge dependences of the boundstate wave functions are dictated. We raise two questions of practical and physical interest, and provide answers to them.

1 Introduction

Recently there has been much progress in our theoretical understanding of nonrelativistic QED and QCD (NRQED and NRQCD) boundstates such as positronium, Υ and remnant of toponium boundstates [1–10]. A notable characteristic in these new developments is that the conventional Bethe-Salpeter equation is no longer being used to calculate the spectrum and wave functions of boundstates. Instead, one starts from the non-relativistic Schrödinger equation (of quantum mechanics) with the Coulomb potential. Then one adds to the nonrelativistic Hamiltonian relativistic corrections and radiative corrections as perturbations to obtain an effective Hamiltonian (quantum mechanical operator) valid up to a necessary order of perturbative expansion. Effective Hamiltonians used in these new formalisms are known to be dependent on the choice of gauge.

We report here our recent achievements [11] on investigations of gauge dependence of a nonrelativistic boundstate formalism used in contemporary calculations. Our motivations for the study are: (I) In the present frontier calculations of higher order corrections to physical quantities of boundstates, often the Feynman gauge is used to calculate typically ultraviolet radiative corrections whereas the Coulomb gauge is used to calculate corrections originating typically from infrared regions. Therefore, it is desirable to clarify gauge dependences of the formalisms actually used in these calculations. (II) We would like to find transformations of boundstate wave functions when we change the gauge-fixing condition. We may apply these transformations to study vari-

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ous amplitudes involving boundstates. Since a physical amplitude is gauge independent, once we know how the wave function transforms, we know how other parts of the amplitude should transform to cancel gauge dependence as a whole. This would provide a useful cross check for identifying all the contributions that have to be taken into account at a given order of perturbative expansion.

A formal argument of gauge dependence/independence of boundstate formalisms goes as follows. It is well known that a quark-antiquark boundstate contributes a pole to the quark-antiquark 4-point Green function:

$$G(p\,qP) = \frac{i}{2\omega_{\nu,\vec{P}}} \frac{\chi_{\nu,\vec{P}}(p)\overline{\chi}_{\nu,\vec{P}}(q)}{P^0 - \omega_{\nu,\vec{P}} + i\epsilon} + (\text{regular as } P^0 \to \omega_{\nu,\vec{P}}), \tag{1}$$

An infinitesimal deformation of the gauge-fixing function in the QCD Lagrangian, $F \to F + \delta F$, induces a variation

$$\int d^4x\, \delta\mathcal{L} = \{iQ_B, \delta\mathcal{O}\}, \qquad \delta\mathcal{O} \equiv \int d^4x\, \mathrm{tr}[\bar{c}\,\delta F]. \tag{2}$$

Any physical amplitude $\langle f;\mathrm{out}|i;\mathrm{in}\rangle$ which involves the quark-antiquark boundstate contributions includes the above Green function $G(pqP)$ as a part of it. Since the initial and final states satisfy the physical state conditions $Q_B\,|\,i;\mathrm{in}\,\rangle = Q_B\,|\,f;\mathrm{in}\,\rangle = 0$ and the theory is BRST invariant, the amplitude is gauge independent. Hence, the boundstate poles included in the amplitude are also gauge independent.

Nevertheless we may raise two intriguing questions: (I) Does the Green function $G(pqP)$ include any unphysical pole, which does not contribute to the physical amplitude, close to or degenerate with one of the physical boundstate poles? A typical example is the R_ξ-gauge for electroweak interaction where an unphysical pole $(k^2 - \xi M_W^2 + i\epsilon)^{-1}$ is included in the gauge boson propagator. (II) Is the boundstate wave function a physical observable? The answer is obviously no since the wave function is gauge dependent as a consequence of the gauge dependence of the effective Hamiltonian. Then, what is the (gauge-independent) physical quantity which can be thought as a counterpart of a boundstate wave function?

We will answer to these questions below.

2 Effective Hamiltonian and Transformation Charge

Let us sketch the outline of our argument. The quantum mechanical Hamiltonian is determined from perturbative QCD order by order in expansion in $1/c$

(inverse of the speed of light):

$$\hat{H} = \hat{H}_0 + \frac{1}{c}\,\hat{H}_1 + \frac{1}{c^2}\,\hat{H}_2 + \cdots . \tag{3}$$

Since quark and antiquark inside a heavy quarkonium are non-relativistic, the expansion in $1/c$ leads to a reasonable systematic approximation. Presently the Hamiltonian is known up to $\mathcal{O}(1/c^2)$. There exist several different definitions of an effective Hamiltonian for the NRQCD boundstates beyond leading order. We introduce an effective Hamiltonian defined naturally in the context of time-ordered (or "old-fashioned") perturbation theory of QCD. Then we obtain a transformation charge Q (quantum mechanical operator) such that the effective Hamiltonian and the boundstate wave function change as

$$\begin{aligned} &\delta H_{\rm eff}(P^0) = \left[H_{\rm eff}(P^0) - P^0 \right] \, iQ(P^0) - iQ^\dagger(P^0) \, \left[H_{\rm eff}(P^0) - P^0 \right], \\ &\delta\varphi = -i\, Q \cdot \varphi \end{aligned}$$

when the gauge-fixing condition is varied infinitesimally. Written in terms of the BRST charge and the field operators in the QCD Lagrangian, Q is given by

$$\begin{aligned} &\left\langle \vec{p}, -\vec{p}, \lambda, \bar{\lambda} \,\middle|\, Q(P^0) \,\middle|\, \vec{q}, -\vec{q}, \lambda', \bar{\lambda}' \right\rangle \\ &= \int \frac{d^3\vec{q}\,'}{(2\pi)^3} \sum_{\lambda'', \bar{\lambda}''} \left\langle \vec{p}, -\vec{p}, \lambda, \bar{\lambda} \,\middle|\, Q_B \, \frac{1}{P^0 - H + i\epsilon} \, \delta O \, \frac{1}{P^0 - H + i\epsilon} \,\middle|\, \vec{q}\,', -\vec{q}\,', \lambda'', \bar{\lambda}'' \right\rangle \\ &\qquad\qquad \times \mathcal{G}^{-1}(\vec{q}\,', \vec{q}; \lambda'', \bar{\lambda}'', \lambda', \bar{\lambda}'; P^0). \end{aligned}$$

Gauge independence of the spectrum can be shown using the transformation. Since Q has no pole $\sim (E - M_\nu + i\epsilon)^{-1}$, there is no unphysical state which contributes a pole to the Green function $\mathcal{G}$ that is degenerate with or close to one of the poles of the physical boundstates of our interest. Stating more explicitly, there is no unphysical boundstate with a binding energy $\sim \alpha_S^2 m$.

3 Application

It is known that the top quark momentum distribution in the $t\bar{t}$ threshold region at leading order is proportional to the absolute square of the wave functions of (would-be) toponium boundstates in momentum space [12]. The momentum distribution will be measured at future collider experiments, so we will be able to probe the boundstate wave functions. As we have shown in Ref.[11], wave functions of boundstates are gauge dependent beyond leading order. We verified that this gauge dependence is cancelled by that of the

final-state interaction diagrams at $\mathcal{O}(1/c)$ when calculating the top quark momentum distribution. In other words, a boundstate wave function mixes with the final-state interaction diagrams by gauge transformation.

Physically b quark emitted in top decays carries the color charge and inevitably interacts with the gluons which were also responsible for the boundstate formation. Since the top quark momentum is reconstructed from the momenta of its offsprings, it is natural that the QCD interaction of the offsprings mixes via gauge transformation in the determination of top momentum distribution.

At the same time, this shows that the present calculations[13] of the top momentum distribution at $\mathcal{O}(1/c^2)$ are gauge dependent, i.e. they vary if we transform the gauge infinitesimally from the Coulomb gauge, since they do not include the final-state interaction diagrams. The example at $\mathcal{O}(1/c)$ suggests how gauge cancellations should take place in the complete amplitude at $\mathcal{O}(1/c^2)$ which has not been obtained yet.

4 Summary

- We used the BRST symmetry to formulate our arguments, which enabled us to discuss gauge dependence of the NRQCD boundstate formalism rigorously.

- Presently, there exist several different definitions of an effective Hamiltonian beyond leading order. We introduced an effective Hamiltonian defined naturally in the context of time-ordered (or "old-fashioned") perturbation theory of QED/QCD. Then we obtained a transformation charge Q (quantum mechanical operator) when the gauge-fixing condition is varied infinitesimally. Also, gauge independence of the spectrum is shown using the transformation.

- For illustration: (1)we calculated the transformation charge Q at next-to-leading order; (2)we demonstrated gauge cancellations among diagrams by examining an infinitesimal gauge transformation of the amplitude for a $q\bar{q}$ boundstate decaying into $q'\bar{q}''W^+W^-$. From the latter example, one can deduce that the present calculations of the top momentum distribution in the $t\bar{t}$ threshold region at next-to-next-to-leading order are gauge dependent.

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